## **XT Parallel 10**

NCCS USERS MEETING



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## **Outline**

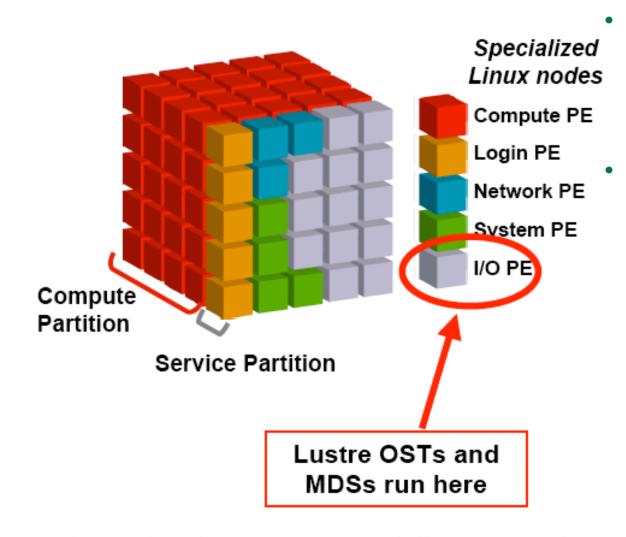
- Jaguar Lustre overview
  - System architecture
  - Lustre Terminology
  - Commands
  - Limitations
- Brief Endian-ness discussion
- Parallel I/O at scale
  - Basic parallel I/O methods
  - Problem with typical methods
  - A solution
  - Benchmarks
- Research



# **Jaguar Lustre overview**

- System architecture
- Lustre Terminology
- Commands
- Limitations

## **Jaguar XT3/4 Architecture**



- Compute partition has
  - 11,508 AMD dual-core processors
  - 46 TB of memory
- Lustre filesystems
  - Serviced by 80 I/O nodes
  - /lustre/scr144
    - 144 OSTs
    - Peak is 72 GB/s
    - Practical ~48 GB/s
    - Early results
      - Read 45 GB/s
      - Write 25 GB/s
  - /lustre/scr72[a,b]
    - 72 OSTs each
    - Default scratch



# **Lustre terminology**

- The concept of object storage is basic to Lustre
  - Objects can be thought of as inodes and are used to store file data. Lustre inodes simply contain references to the object storage target (OST) that stores the file data
  - Access to these objects occurs through object storage servers (OSSs), which provide the file I/O service
  - The OSTs perform the block allocation for data objects, which results in distributed and scalable allocation

# **Lustre terminology (cont.)**

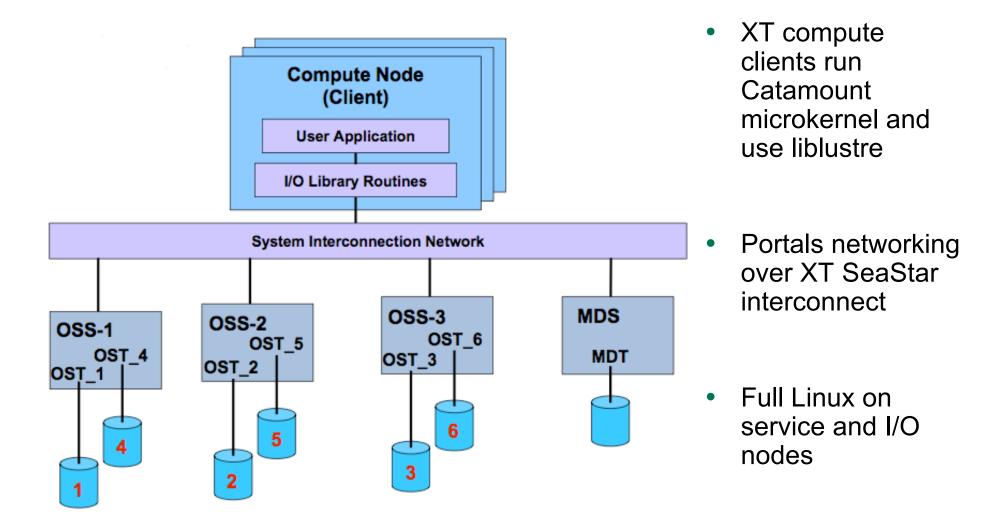
- The namespace is managed by metadata services that manage the Lustre inodes
  - The services perform file lookups, file creation, file and directory attribute manipulation
  - Such inodes can be directories, symbolic links, or special devices
  - The associated data and metadata is stored on the metadata servers

# **Lustre terminology (cont.)**

- MDS metadata server
  - The Server node
- MDT metadata target
  - This is the software interface to the backend volume
  - Controls filesystem metadata (inodes) and locking mechanism
    - The backend volume is an ext3 file system
    - LUNs are formatted with 4096 byte blocks
- OSS object storage server
  - The server node
  - Support multiple OSTs
- OST object storage target
  - This is the software interface to the backend volume
    - The backend volume is an ext3 file system
    - LUNs are formatted with 4096 byte blocks
    - The multi-block allocator (MBA) (Linux 2.6) is used for performance
    - LUN size is limited to 2 TB



#### **XT3/4 Lustre Architecture**



#### **Lustre commands**

- Ifs Lustre utility that can be used to create a file with a specific striping pattern, displays file striping patterns, and find file locations
  - Suboptions: setstripe, getstripe, find, help
- Examples
  - set stripe width (count) to 1 on <dir>
    - lfs setstripe <dir> 0 -1 1
  - find stripe width on <filename> with minimal output
    - lfs find --quiet <filename>
  - find stripe width on <filename> with default output
    - lfs getstripe <filename>
  - Set stripe size (per striped OST) to 2MB on <dir>
    - lfs setstripe <dir> 2097152 -1 1
  - Get online help
    - lfs help <suboption>



### **Lustre limits**

- The maximum file size is 320 TB (on any lustre)
  - Maximum number of stripes per file is 160
    - 2 TB x 160 = 320 TB (2 TB is max LUN size)
- Limits on Jaguar

Limits	Max Stripe count	Capacity
/lustre/scr144	144	288 TB
/lustre/scr72[a,b]	72	144 TB

- scr72a and scr72b don't overlap
- scr72[a,b] overlaps half of scr144

#### **Endian-ness**

- Little-endian
  - x86 machines (Intel, AMD), DEC Alpha
    - XT3/4
- Big endian
  - X1[E], IBM PPC (including BG/L), MIPS, Sparc
- Many compilers provide bi-endianness support for Fortran binary files (Intel, PGI, etc)
  - But is there a price to pay?

#### **Endian-ness**

- One can use the PGI -byteswapio option to swap the endian-ness for Fortran I/O
  - You can use this on a subroutine by subroutine basis
- Creating a 4GB file (512 8MB writes) with one process, sequential unformatted (on XT3)
  - Default: ~18 MB/S
  - byteswapio: ~9.4 MB/s
- User called endian swap
  - Can get ~15 MB/s
  - \*\* But control words will be different endian-ness than the data
- Very similar results using direct unformatted (simulating sequential I/O)

### **Endian-ness discussion**

- So there is a cost (50%) when doing Fortran unformatted I/O with one process
  - Can this cost be amortized away in parallel?
  - With 100 or more processes, the cost is reduced to ~23% hit
    - 96 processes in SN mode writing 16 MB each
      - default 7.1 GB/s
      - byteswapio 5.4 GB/s
    - 192 processes in VN mode writing 16 MB each
      - default 11.7 GB/s
      - byteswapio 9.2 GB/s
- This may matter if the I/O cost in your code is significant

### Parallel I/O at scale

- Basic parallel I/O methods
  - Problem with typical methods
  - A solution
- Benchmarks
  - Striping
  - Buffer sizes
  - Subsetting

# Parallel I/O in general

- Two common methods:
  - All data is reduced to 1 process which does I/O
  - All tasks do I/O
    - A file read/written by each task
      - Independent files
    - All tasks read/write a part of one file
      - shared file
- With both methods, typically one uses
  - Fortran or C I/O with MPI
    - Records/seeks for shared file
  - MPI I/O
  - Parallel HDF5 or netCDF
    - won't be talking about these today

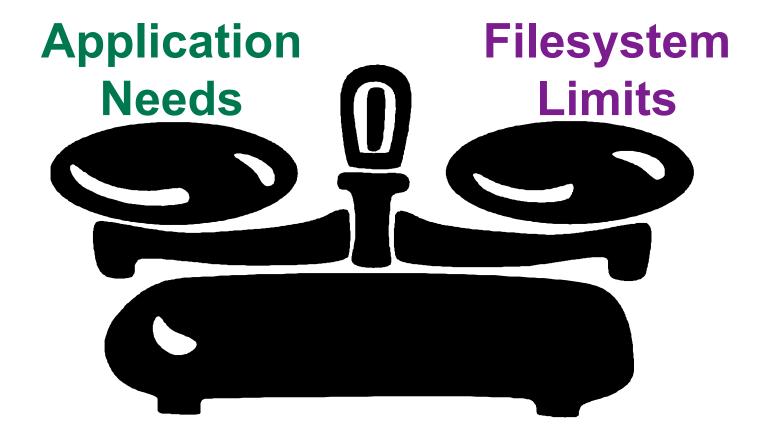


#### **The Problem**

- These methods are fine until you scale-up
  - Proof forthcoming
- Without user-intervention you will not get practical peak
   I/O bandwidth
- For example
  - Single writer/reader reduction
    - Even with maximum striping on file, effective bandwidth is limited by the 1 compute node (200 MB/s)
  - All processes read/write at the same time
    - Slow opens (all hit the MDS at the same time)
    - Overwhelm OSTs and/or IO service nodes
    - Possibly inconvenient to users



## **Striking a Balance**



### **Subset of readers/writers**

- The Plan:
  - Combine the best of our first two I/O methods
  - Choose a subset of nodes to do I/O
  - Send output to or Receive input from 1 node in your subset
- The Benefits
  - I/O Buffering
  - High Bandwidth, Low FS Stress
- The Costs
  - I/O Nodes must sacrifice memory for buffer
  - Requires Code Changes



## Subset of readers/writers (cont.)

- Assumes job runs on thousands of nodes
- Assumes job needs to do large I/O
- From data partitioning, identify groups of nodes such that:
  - each node belongs to a single group
  - data in each group is contiguous on disk
  - there are approximately the same number of groups as OSTs
- Pick one node from each group to be the ionode
- Use MPI to transfer data within a group to its ionode
- Each IO node reads/write shared disk file



## **Example code**

create an MPI communicator that include only ionodes;

listofionodes is an array of the ranks of writers/readers

```
call MPI_COMM_GROUP(MPI_COMM_WORLD, &
    WORLD_GROUP,ierr)

call MPI_GROUP_INCL(WORLD_GROUP,nionodes, &
    listofionodes,IO_GROUP,ierr)

call MPI_COMM_CREATE(MPI_COMM_WORLD,IO_GROUP, &
    MPI COMM_IO,ierr)
```

## **Example code (cont.)**

```
open
  call MPI FILE OPEN (MPI COMM IO, trim (filename), &
       filemode, finfo, mpifh, ierr)
read/write
  call MPI FILE WRITE AT (mpifh, offset, iobuf, &
        bufsize, MPI REAL8, status, ierr)
      OR
  call MPI FILE SET VIEW (mpifh, disp, MPI REAL8, &
        MPI REAL8, "native", MPI INFO NULL, ierr)
  call MPI FILE WRITE ALL (mpifh, bigA, size (bigA), &
        MPI REAL8, status, ierr)
close
  call MPI FILE CLOSE (mpifh, ierr)
```

## **Benchmarks**

- Topics discussed
  - Lustre striping
  - Buffer sizes
  - Subsetting

## **Caveats**

- OS level not consistent for all tests
  - Striping tests done with 1.5.25
  - Some with 1.5.29 and others with 1.5.31
- Some results from XT3 and some from XT4
- Some runs done in dedicated mode
- And others done during regular production usage
  - For these, we report the "max" time over many trials sort of a practical peak

# **Striping**

- Lustre has the flexibility to specify how a file is striped across OSTs
  - Default set when file system is made
  - User can specify with Ifs setstripe [dir I file] ...
- Striping across multiple OSTs is useful when an application writes large, contiguous chunks of data
  - OSTs run in parallel, increasing I/O performance
- If the application isn't writing large data, striping will hurt
  - Don't stripe for small files



## **Benchmark Results: 1 I/O Node - Stripes**

 Single IO node, 10 megabyte buffer, 20 megabyte stripe size: bandwidth of IO write to disk

#### Number of stripes

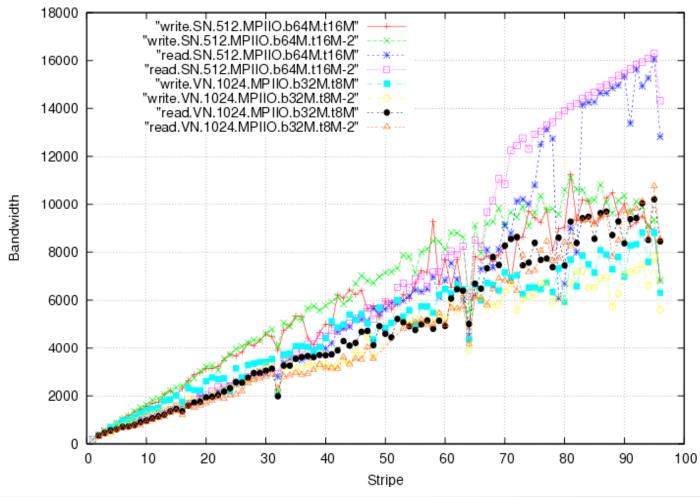
```
1 10 50 100 150 160
150MB/s 134MB/s 135MB/s 139MB/s 149MB/s 148MB/s
```

- Using a single IO node:
  - number of stripes doesn't matter
  - stripe size doesn't matter (timings not shown)



## XT3 Striping, lustre 1.5.25, 96 OSTs





## **Striping discussion**

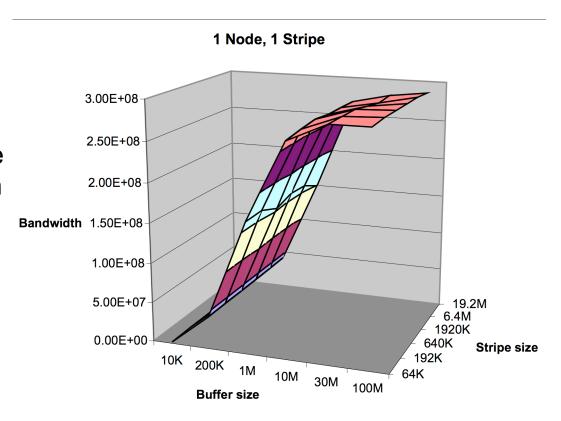
- From the data, we see
  - Don't use multiples of 32
  - Don't use max
    - Not sure if this applies to lustre config on XT4?

## **Buffer sizes**



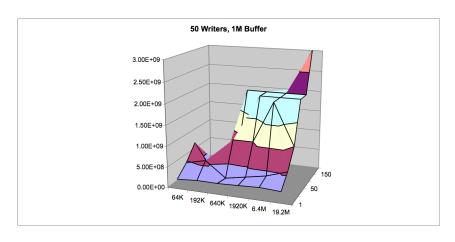
#### **Benchmark Results: 1 I/O Node - Buffer Size**

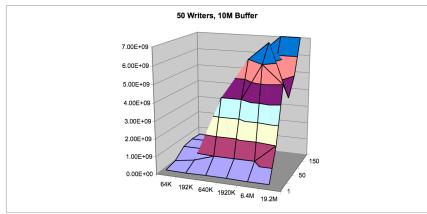
- Single node, single stripe: bandwidth of IO write to disk for different buffer sizes
  - Buffer size is the size of contiguous memory on one IO node written to disk with one write
- Buffer size should be at least 10 megabytes

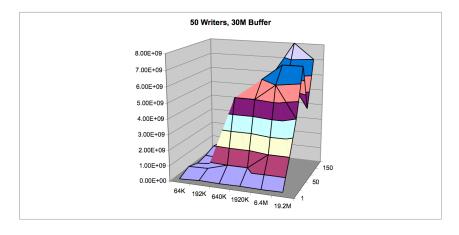


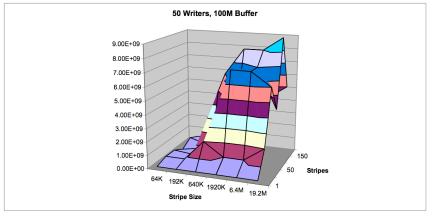


# 50 Writers, Varying Stripe Count, Size and Buffer Size

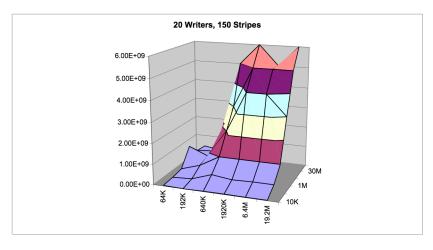


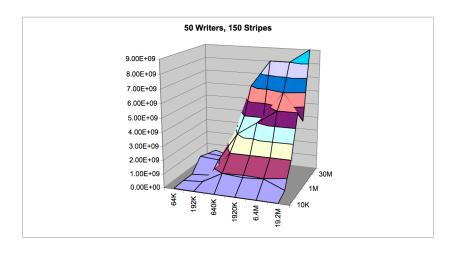


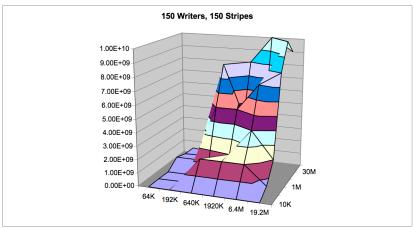


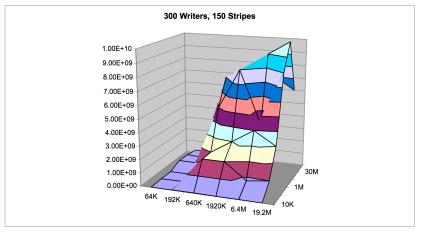


# 150 Stripes, Varying Writers, Buffer, and Stripe Sizes









## **Scaling clients**

- Will now show benchmark data of scaling the number of IO clients, with
  - Custom MPI/Fortran code
  - IOR

## **Parallel Fortran I/O**

•10 MB file per process

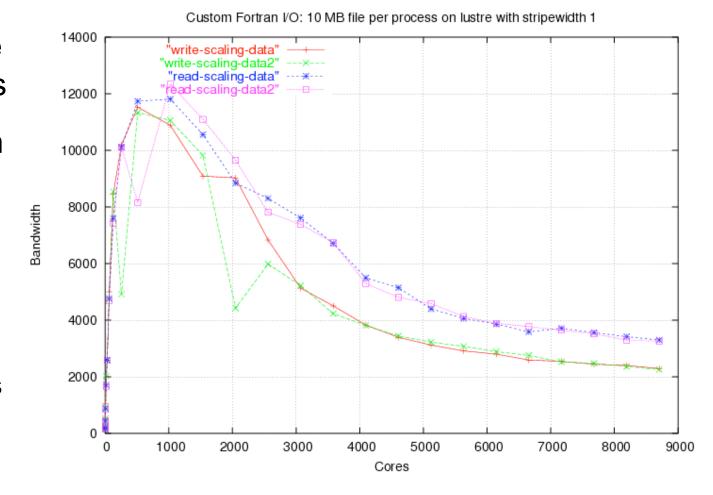
stripewidthof 1

•XT3

•1.5.29

•pgi/6.1.4

•96 OSTs



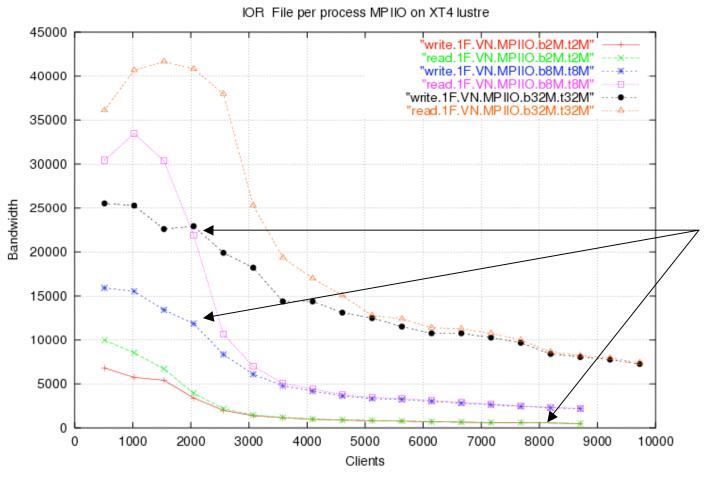


# Parallel Fortran I/O (cont.)

- This plot tells us ....
  - Sweet spot around 512-1024 writers
  - At full size
    - 2 GB/s writes, 3 GB/s reads
  - Reads faster than writes >= 1024 writers

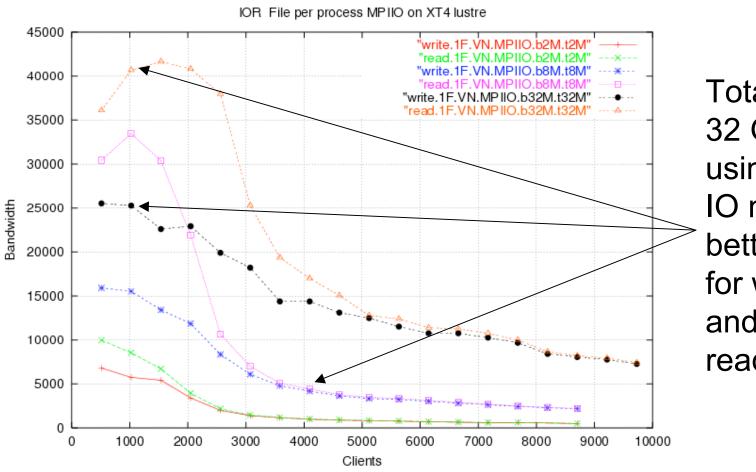
\* Data taken in non-dedicated mode

# XT4, 1.5.31, pgi/6.2.5, 144 OSTs



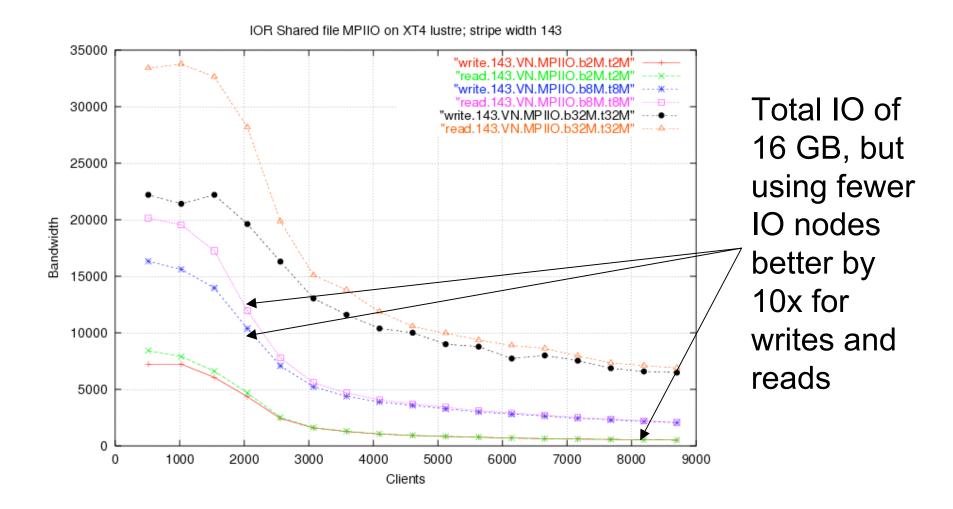
Total IO of 16 GB, but using fewer IO nodes better by 10x for writes and 20x for reads

# XT4, 1.5.31, pgi/6.2.5, 144 OSTs

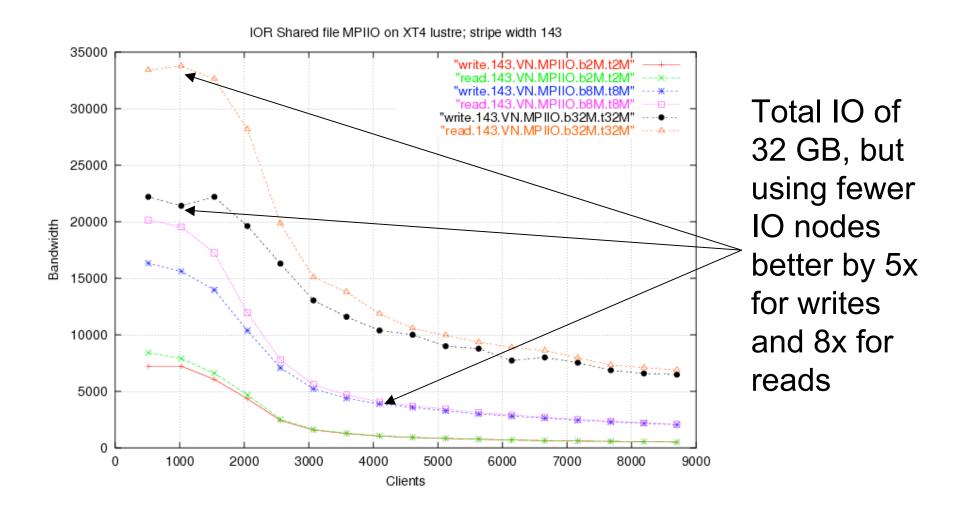


Total IO of 32 GB, but using fewer IO nodes better by 5x for writes and 8x for reads

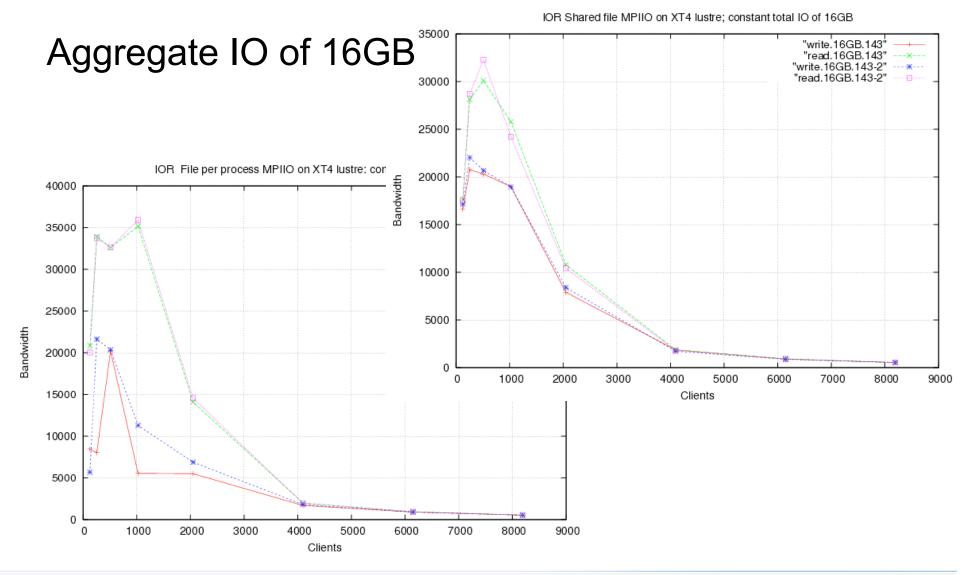
# XT4, 1.5.31, pgi/6.2.5, 144 OSTs



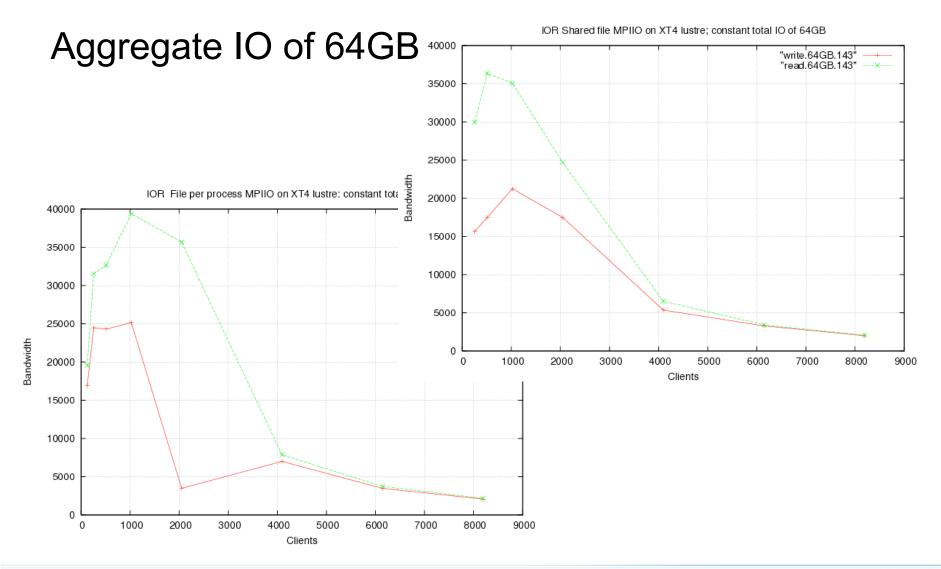
# XT4, 1.5.31, pgi/6.2.5, 144 OSTs



# XT4, 1.5.31, 144 OSTs



# XT4, 1.5.31, 144 OSTs



# **IOR** scaling results

- These plots tell us ....
  - Larger IO buffers are better
  - Using fewer IO nodes at large scale is better
    - Optimal # of IO nodes is dependent on IO buffer size, data suggests
      - 2-8 x (# of OSTs) for 16GB aggregate file IO
      - 4-8 x (# of OSTs) for 64GB aggregate file IO

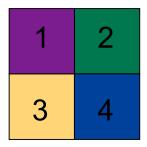
# Writer/Reader Subsetting

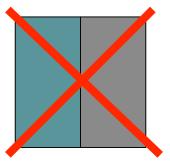
- On ORNL's XT3 and XT4, sufficient evidence to conclude that too many readers/writers degrades IO bandwidth
  - Since the optimal number of IO nodes looks to be somewhere around 1024, we believe that using a subset of clients for IO is beneficial
- Goal: use subset of MPI processes to do IO
  - Shown to be more effective in previous slides
  - Aggregates IO too
  - Can't MPI IO does this automatically with hints?
    - Still investigating on XT
- Note: I have seen one plot (in a lustre tutorial class) of data from Sandia's Red Storm that shows almost no degradation from 2K clients out to 10K clients (40GB/s)
  - Unable to repeat this



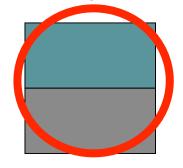
### **Sample Partitioning: POP**

- data is 3d X, Y, Z
- X and Y dimensions are partitioned in blocks
- sample 4 node partition:
  - Each of the 4 colored blocks represents one node's part of the data
  - Each of the two lighter colored blocks represent 1 I/O Node
  - I/O Groups should be arranged so their data is contiguous on disk





Data from nodes 1 & 3 alternate on disk. This will perform slowly and can't adjust to more processors.



Data from node 1 is contiguous, followed by data from node 2, which is also contiguous.



### **Sample Partitioning: POP**

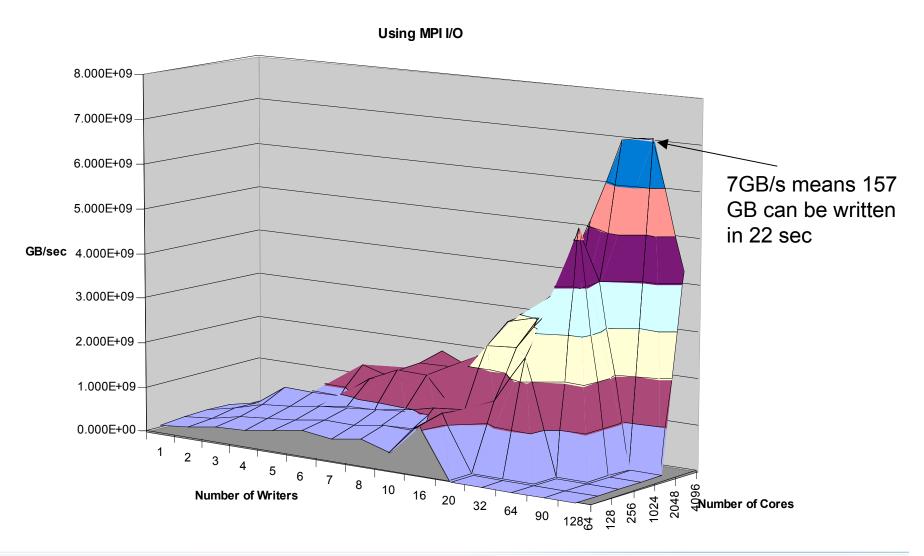
- Given a nearly square partitioning, the number of nodes simultaneously performing IO is approximately the square root of the total number of compute nodes.
  - 2500 compute nodes 50 IO nodes
  - 10000 compute nodes 100IO nodes
  - 25600 compute nodes 160 IO nodes
- Many partitions allow a reasonable assignment of ionodes

#### For Example:

- An array of 8 byte reals (300, 400, 40) on each of 10000 nodes
  - 4.8 million elements on each node
  - 48 billion elements total
  - 384 gigabytes data
  - 50 100 seconds to read or write at 4 8 gbyte/sec
  - 100 IO nodes



#### **A Subset of Writers Benchmark**



### **Benchmark Results: Things to Know**

- Uses write\_at rather than file partitioning
- Only write data...sorry
  - Read data was largely similar
- Initial benchmarking showed MPI transfers to be marginal, so they were excluded in later benchmarking
- Real Application Data in the works, Come to CUG

# **Subsetting Example 2**

- Jan test on XT3 with 1.5.29 (non-dedicated test), 96 OSTs
- Custom code (used earlier for scaling plot)
  - 1 file per proc (stripe width 1); 8640 processes (cores)
  - Will have it use a subset of the procs as ionodes
    - Can aggregate data or serially send data to ionodes
- Test1: 5 MB writes/reads (smaller buffer)
  - With 8640 writers
    - Writes: 1.4 GB/s; Reads: 2.0 GB/s (max of 2 runs)
  - With 960 writers, aggregating data on writers
    - Writes: 10.1 GB/s; Reads: 10.3 GB/s (max of 2 runs)
- Test2: 10 MB writes/reads (same buffer)
  - With 8640 writers
    - Writes: 2.3 GB/s; Reads: 3.1 GB/s (max of 2 runs)
  - With 960 writers, aggregating data on writers
    - Writes: 7.2 GB/s; Reads: 9.0 GB/s (max of 2 runs)



# **Subsetting Example 3**

- XT4, 1.5.31, 144 OSTs, pgi/6.2.5
- Only Test (so far): 8 MB writes/reads
  - With 9216 writers
    - Writes: 619 MB/s (not as good as XT3)
  - With 1024 writers, serially sending data to writers
    - Writes: 10.4 GB/s

#### **Take Home Notes**

- Do Large I/O Operations in Parallel with MPI-IO
- Create a natural partitioning of nodes so that data will go to disk in a way that makes sense
- Stripe as close to the maximum OSTs as possible given your partitioning
- Use buffers of at least 1MB, 10MB if you can afford it
  - On XT, try IOBUF I/O buffering layer
    - It works and requires no code changes
      - Can buffer stdout too
    - Loaded by default, "man iobuf" for more information
      - Typically can improve upon default settings
- Make your I/O flexible so that you can tune to the problem and machine
  - One hard-coded solution will meet your needs some of the time, but not all of the time
  - Use a subset of IO nodes (make this tunable) when running large-scale
    - According to recent tests, 4-8 x the number of OSTs
  - MPI I/O hints would be a portable solution (need to verify it works on XT)



### **Take Home Notes (cont.)**

- On parallel HDF5 and parallel-netCDF
  - General consensus at Cray Technical Workshop is that they perform very poorly, lustre or not.
    - I know this is not what you want to hear
  - People are working on it
- Everyone opening a file at the same time at scale is sure to be slow, offset if possible
- Performance will be variable
  - Lustre filesystem is a shared resource



#### **Other**

- Be aware of distribution of files across OSTs
  - If you do one file per process, make sure this distribution is equal across OSTs
    - lustre gets the distribution even or very close,
    - But if run with 8 procs, and then 16, and then ....
      - Sometimes you will not get even distribution across the OSTs
    - Even if you "replace" each file during a checkpoint, they will end up in the same OST
  - For small scale (< #ofOSTS), if one OST is used twice, it flatlines your scaling
  - Sometimes easiest to remove all files and then recreate them



### **Current Research**

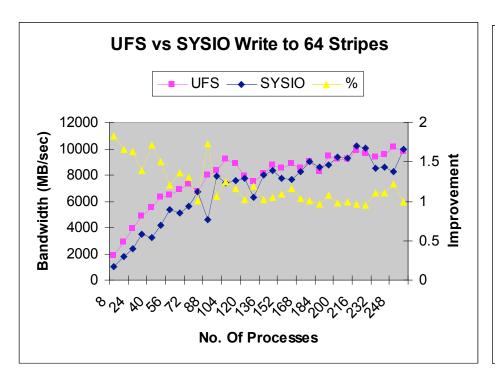
### **Parallel IO Instrumentation**

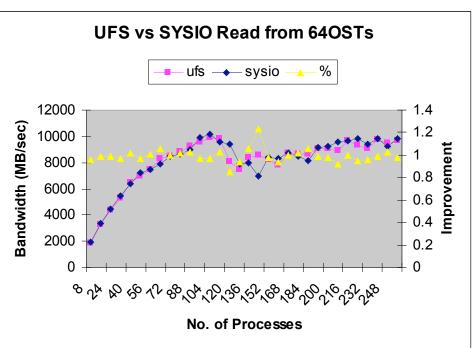
- Default Parallel IO over XT3/4
  - ROMIO implementation over libsysio
  - Include Cray optimizations but proprietary code base
  - Hard for code dissection and performance analysis
- Creating a different parallel IO stack over XT3/4:
  - ROMIO over UFS
    - UFS-based ROMIO is applicable because Lustre is Posix compliant
  - Initial performance testing with IOR
  - Performance profiling with collective IO



### **ROMIO** over UFS

- Performance with ROMIO over UFS
  - Write can be up 80% more efficient
  - Read is comparable, within 1%





-- Weikuan Yu at ORNL



# **Parallel IO Timing Profiling**

- Why is collective IO slow?
  - Significant time spent in collective communication, and growing
  - What this tells us:
    - Communication is a scalability limiter inside collective IO
    - Do not forget hints to avoid collective communication if your output from large, contiguous, and non-overlapping regions

# Timing Breakdown of Collective IO on XT --Weikuan Yu at ORNL

Nprocs	Collective Comm	File IO	Comm/IO Ratio
IOR (millisec)			
16	5210.87	22880.90	.23
32	13204.93	45290.90	.29
64	32034.95	89522.71	.36
Flash IO Checkpoint file (millisec) – PNetCDF version			
16	2872.84	2469.78	1.16
32	5696.86	4371.18	1.30
64	12019.0	8096.6	1.48



# What's Expected Soon?

- Upcoming Results
  - Attend CUG 2007 for Parallel IO stack efficiency over XT3/4
    - HDF5
    - Parallel NetCDF
    - MPI-IO
    - Fortran and Unix IO
  - With working examples on what tunables (hints) to use and how to use them over XT3/4 for these stacks.
- Upcoming optimizations
  - Exploit Lustre file joining, prototyped over Linux-based platforms
  - Explore overlapped communication and IO
  - Explore more scalable collective communication for IO



# **Documentation/help**

- See Cray Docs at <a href="http://docs.cray.com">http://docs.cray.com</a>
  - XT Programming Environment User's Guide
    - IOBUF and other buffering techniques
  - Lustre reference manual
  - Also see these man pages
    - Strided I/O functions: readx, writex, ireadx, iwritex
- See <a href="http://info.nccs.gov/resources/jaguar">http://info.nccs.gov/resources/jaguar</a>
  - http://info.nccs.gov/resources/jaguar/iotips
- Much of this will be on the jaguar iotips page soon!
- Contact your liaison or <a href="mailto:help@nccs.gov">help@nccs.gov</a> if you need help optimizing your IO



# **Acknowledgements**

- XT architecture picture from "Cray and Lustre" talk by Carroll and Radovanovic at CUG06.
- Lustre architecture picture from "Lustre tutorial" given by R. Slick at CUG06.
- Lots of material taken from "Efficient I/O on the Cray XT" talk by J. Larkin at Cray Technical Workshop, Feb 07.
- The "Current Research" material provided by Weikuan Yu.